Pentadecane, 2-methyl-

Other names: 2-Methylpentadecane
Inchi: InChI=1S/C16H34/c1-4-5-6-7-8-9-10-11-12-13-14-15-16(2)3/h16H,4-15H2,1-3H3
InchiKey: BANXPJUEBPWEOT-UHFFFAOYSA-N
Formula: C16H34
SMILES: CCCCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 226.44
CAS: 1560-93-6

Physical Properties

Property code	Value	Unit	Source
gf	81.40	kJ/mol	Joback Method
hf	-378.85	kJ/mol	Joback Method
hfus	33.67	kJ/mol	Joback Method
hvap	50.82	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	6.344		Crippen Method
mcvol	236.300	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	1561.00		NIST Webbook
rinpol	1564.89		NIST Webbook
rinpol	1564.84		NIST Webbook
rinpol	1563.71		NIST Webbook
rinpol	1564.10		NIST Webbook
rinpol	1564.13		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1564.80		NIST Webbook
rinpol	1565.20		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1569.00		NIST Webbook

rinpol	1566.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1564.10		NIST Webbook
rinpol	1564.00		NIST Webbook
tb	565.04	K	Joback Method
tc	726.28	K	Joback Method
tf	262.40 ± 2.00	K	NIST Webbook
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.96	J/mol×K	565.04	Joback Method
cpg	650.21	J/mol×K	618.79	Joback Method
cpg	668.20	J/mol×K	645.66	Joback Method
cpg	685.47	J/mol×K	672.53	Joback Method
cpg	702.03	J/mol×K	699.40	Joback Method
cpg	717.90	J/mol×K	726.28	Joback Method
cpg	631.47	J/mol×K	591.91	Joback Method
dvisc	0.0022640	Pa×s	306.74	Joback Method
dvisc	0.0009470	Pa×s	358.40	Joback Method
dvisc	0.0004934	Pa×s	410.06	Joback Method
dvisc	0.0002974	Pa×s	461.72	Joback Method
dvisc	0.0001985	Pa×s	513.38	Joback Method
dvisc	0.0001427	Pa×s	565.04	Joback Method
dvisc	0.0077044	Pa×s	255.08	Joback Method
hvapt	62.00	kJ/mol	485.50	NIST Webbook
rhol	754.10	kg/m3	323.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	761.00	kg/m3	313.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels

rhol	767.90	kg/m3	303.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	774.90	kg/m3	293.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	781.80	kg/m3	283.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	718.90	kg/m3	373.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	726.00	kg/m3	363.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	733.00	kg/m3	353.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels
rhol	740.00	kg/m3	343.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels

rhol	747.00	kg/m3	333.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels	
rhol	754.00	kg/m3	323.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels	
rhol	761.00	kg/m3	313.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels	
rhol	768.00	kg/m3	303.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels	
rhol	775.00	kg/m3	293.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels	
rhol	782.20	kg/m3	283.15	Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels	

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42741e+01
Coeff. B	-4.21040e+03
Coeff. C	-1.18700e+02
Temperature range (K), min.	419.73
Temperature range (K), max.	588.47

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol173.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1560936&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Density, Viscosity, Speed of Sound, and Bulk Modulus of Methyl Alkanes, Dimethyl Alkanes, and Hydrotreated Renewable Fuels:	https://www.doi.org/10.1021/je400274f
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume